MEANS

Final Report

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Microstructure-Based Modeling for Life-Limited Components
AFOSR Grant #F49620-02-1-0056

Preamble

The principle objective of the project was to bring together computational and experimental efforts in a comprehensive program to develop an integrated set of computational tools that would permit predictions of microstructural development and microstructure-based modeling of life-limited components in advanced titanium alloys (Ti-64 and Ti-6242). These computational tools are anticipated to significantly reduce extensive testing schedules and processing and inspection procedures, and permit development and insertion of new materials within acceptable costs and time frames. This AFOSR support underscored the activities of the Center for Accelerated Maturation of Materials (CAMM) at the Ohio State University (OSU). Significant progress has been made in integrating both experimental and computational efforts and different computational methods, ranging from CALPHAD thermodynamic modeling to phase field microstructure modeling, phenomenological equations, FEM crystal plasticity modeling and neural networks. The MEANS program involved graduate students and postdoctoral fellows in two departments (MSE and Mechanical Engineering) at OSU. Close and highly productive collaborations among the PIs have been established, leading to many publications in leading scientific journals. Moreover, strong interactions have been established between the MEANS and other on-going programs at CAMM, including the AFRL Metal Affordability Initiative (MAI) program and STW-21 program, and its industry partners. The outcomes of the project have made significant impact on developing and incorporating robust, predictive and physics-based materials models into new design philosophy for accelerated maturation and insertion of advanced titanium alloys. The major accomplishments are summarized bellow according to the three tasks, namely the modeling of fatigue in Ti-based alloys, microstructural modeling, and multi-time scale integration method for cyclic deformation in polycrystalline metals.

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14. ABSTRACT

The principle objective of the project was to bring together computational and experimental efforts in a comprehensive program to develop an integrated set of computational tools that would permit predictions of microstructural development and microstructure-based modeling of life-limited components in advanced titanium alloys (Ti-64 and Ti-6242). These computational tools are anticipated to significantly reduce extensive testing schedules and processing and inspection procedures, and permit development and insertion of new materials within acceptable costs and time frames. This AFOSR support underscored the activities of the Center for Accelerated Maturation of Materials (CAMM) at the Ohio State University (OSU). Significant progress has been made in integrating both experimental and computational efforts and different computational methods, ranging from CALPHAD thermodynamic modeling to phase field microstructure modeling, phenomenological equations, FEM crystal plasticity modeling and neural networks. The outcomes of the project have made significant impact on developing and incorporating robust, predictive and physics-based materials models into new design philosophy for accelerated maturation and insertion of advanced titanium alloys.

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Task 1: Modeling of Fatigue in Ti-based alloys

Predictive models have been developed for tensile properties in both α/β and β-processed Ti-6-4. Based upon microstructural inputs, it has been possible to develop Bayesian Neural Network models for the provision of tensile properties based upon a rigorously quantified microstructure [1-5]. This task has focused on leveraging the knowledge from such previous work to determine whether similar techniques can be applied to fatigue lifetimes in Ti-6Al-4V. Techniques included in this work include optical microscopy (*see Fig. 1.1(a)*), electron microscopy, fractography (*see Fig. 1.1(b)*), crack growth rate analysis, stereology (Thickness of Widmanstätten α-laths, colony scale factor, Prior-β grain size factor, Volume Fraction basketweave [1-5]), and fuzzy logic
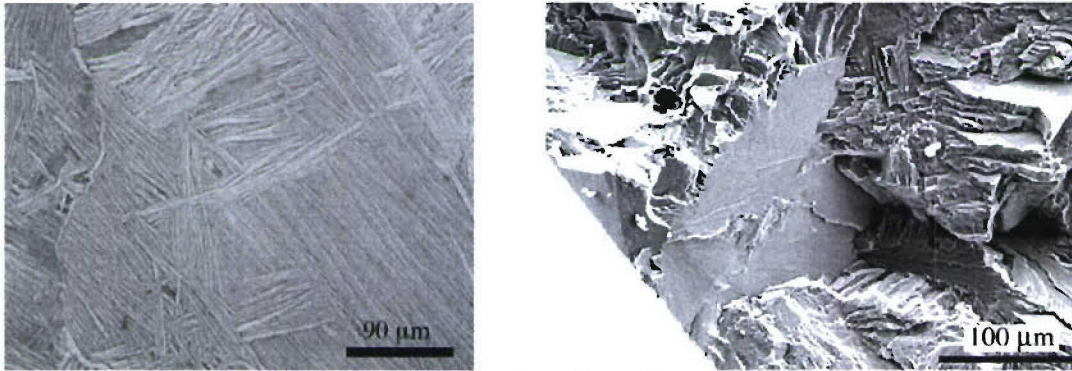

Figure 1.1. (a) Optical micrograph of a representative colony microstructure and (b) fractography showing the surface initiation of a clearly defined crack nucleation region.

models (on 550 MPa tests). S-N type fatigue testing was performed in tension-tension fatigue under load-control conditions at room temperature and in a laboratory air environment. A load ratio of R = 0.10 was used for all tests and the number of cycles to failure was recorded primarily at 3 different stresses: 550, 600, and 675 MPa.

Based upon a calculation of the number of cycles to propagate a crack of $100\mu m^2$ to failure, the minimum lifetime was calculated for each of the stress levels, and is shown as the dashed-line in Fig. 1.2. In this analysis, the fatigue crack growth data is calculated using data reported by R.K. Nalla [6]. The data points in Fig. 1.2 represent the actual lifetimes. It would appear that for the material used in this study, the fatigue crack growth portion of the lifetime provides an accurate approximation for the minimum lifetime. However, at this point in time, this is an estimation, as the variation in microstructural features present (e.g., 0.27 to 0.42 μm for an average α-lath thickness), might effect these calculations. Additionally, the small dataset (26 samples) results in initial results, as expected for the development of a life-based predictive models. Therefore, there is expected to be an uncertainity associated with the models.

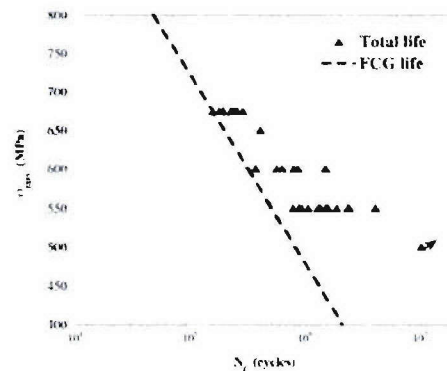It was observed during our initial modeling efforts that plots of microstructural feature vs.

Figure 1.2. Stress vs. lifetime for 30 samples. The dashed line indicates the number of cycles spent growing a crack with an area of $100\mu m^2$ to failure.
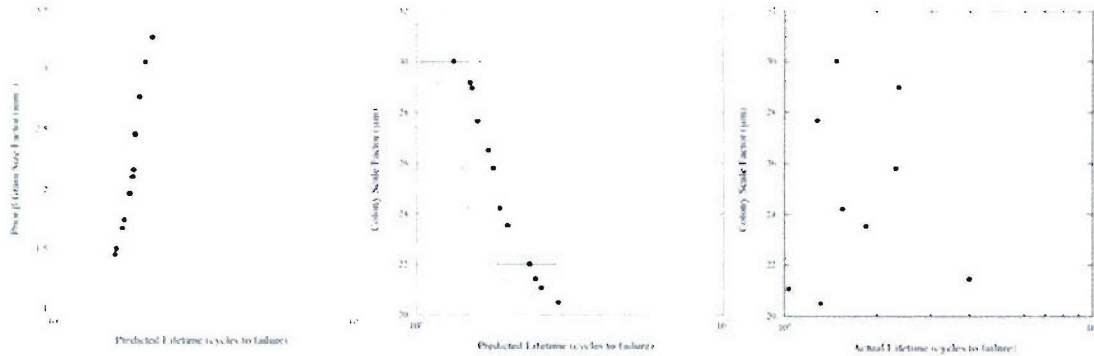
Figure 1.3: Results of fuzzy logic models for the data subset comprised of only the samples tested at 550 MPa showing (a) prior β grain size factor, (b) Colony scale factor and vs. predicted lifetime.and (c) Colony Scale Factor vs actual lifetime.

predicted lifetime seemed to separate out to a certain extent by stress, and that microstructure-property relationships were difficult to identify when stress was used as an input variable. It is believed that using stress as an input parameter into the fuzzy logic models may introduce a complexity that cannot be easily dealt with when working with a relatively small sample population. Therefore, for the remainder program, stress was removed as an input parameter for further modeling experiments, limiting using only the 550 MPa data set, resulting in a limited data set, but one with less error (21.4% vs. 27%).

Selected plots for predicted lifetime vs. microstructural parameter for the specimens tested at 550 MPa are shown in Figures 1.3 (a-c). In Figure 1.3 (b), the trend between colony scale factor and predicted lifetime is clear and indicates that increasing the colony size tends to decrease the lifetime. This would support the observation that colonies tend to serve as the smallest resolvable fatigue crack initiation site for these samples. By comparing Figures 1.3 (b) and 1.3 (c), one can see the usefulness of the fuzzy logic modeling method when investigating microstructure-property relationships for titanium alloys. The model has evaluated the independent effect of colony scale factor on lifetime at a given stress, whereas the data shown in Figure 1.3 (c) (the "raw" data), includes variations in all other microstructural parameters. It is clear that the variation in fatigue lives predicted by the models was smaller than the experimentally measured lives. Thus, it appears that this modeling method will be able to provide a valuable tool for investigating microstructure – property relationships in titanium alloys by providing a capability that empirical methods alone cannot. By using fuzzy logic modeling, one can perform "virtual experiments" that enable one to look at the *independent* effect of a single microstructural feature size on a mechanical property. These results are particularly interesting because a trend, albeit very slight, is seen for colony size vs. fatigue lifetime within a single heat treatment of Ti-6Al-4V, for which the microstructure is nominally constant across all samples. Future work on further microstructural variations of Ti-6Al-4V alloy will be useful for determining the capabilities of this modeling method.

Based on the current research on the fatigue life behavior of as-forged β-processed Ti-6Al-4V, the following salient conclusions can be drawn:

- Minimum lifetimes for this alloy appear to correspond to the number of cycles spent nucleating and propagating a penny-shaped crack with an area of 100 μm^2, which approximated the area of the apparent critical crack initiation site.
- Using fuzzy logic models to analyze the independent effect of one microstructural parameter on the lifetime, the range of predicted lifetimes is shown to be much smaller than the tested values.
- For the samples tested at 550 MPa, a trend is apparent in the plot of colony scale factor vs. predicted lifetime, although the error in the model is still too large to confirm any relationship.

Task 2: Microstructure Modeling

Phase transformation and microstructural evolution in commercial titanium alloys are extremely complex. The traditional constitutive models that characterize microstructural features by average values without capturing the anisotropy and spatially varying aspects may not be sufficient to quantitatively define the microstructure and hence to allow for establishing a robust microstructure-property relationship. In this project we integrate thermodynamic modeling and phase field simulation to develop computational tools for quantitative prediction of phase equilibrium and spatiotemporal evolution of microstructures during thermal processing that account explicitly for precipitate morphology, spatial arrangement and anisotropy. The rendering of the predictive capabilities of the phase field models as fast-acting design tools through the development of constitutive equations is also demonstrated (see Figs. 2.1-2.5 for examples).

By adopting a partnering and leveraging approach with the Air Force Research Laboratory (AFRL) Metals Affordability Initiative (MAI) program, entitled Microstructure and Mechanical Property Model Development for Wrought Titanium Alloys, quantitative modeling tools for the prediction of critical microstructural features as a function of heat-treatment have been developed. These features have been identified as key to LCF and *da/dN*, which include the following

- Beta grain size and texture
- Thickness of grain boundary alpha
- Growth and coarsening of globular alpha
- Precipitation of lamellar alpha (alpha side-plates)

To link the phase field method to the thermodynamic modeling tools developed in the MAI program, including *Pandat*, a software package for multi-component phase equilibrium calculations, and *PanTitanium*, a thermodynamic database for multi-component titanium alloys, local free energy density functions for α/β Ti alloys have been formulated by combining the CALPHAD style free energy functions with the traditional Landau
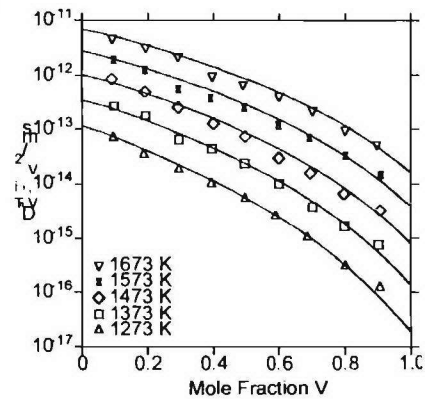
Fig. 2.1. The calculated (lines) and experimental determined (symbols) interdiffusivities in Ti-V system. $\widetilde{D}_{V,V}^{Ti}$ is the interdiffusivity of Ti in V.

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polynomial expansions or the polynomial expansions developed for solidification. In contrast to the intensive efforts devoted to thermodynamic database development, not much attention has been given to the development of mobility databases. As a consequence, multi-component Ti alloys were often treated as pseudo-binary systems. In this project, a mobility database for Ti-Al-V has been established using the DICTRA approach. An example of the interdiffusivities in the Ti-V system predicted by the database is shown in Fig. 2.1, which agrees very well with experimentally determined values. In addition to the phase-field modeling carried out in this project, the assessed mobility data for TI-Al-V are also crucial in modeling solidification, homogenization, bonding, protective coating, creep and other diffusion-related processes.

With these integrations, quantitative material-specific phase field models have been developed and applied to characterize grain boundary α thickening (Fig. 2.2), growth and dissolution of globular α (Fig. 2.3), formation and growth kinetics of α sideplates (Fig. 2.4), and the competition between sideplate colonies and basketweave structures (Fig. 2.5) in Ti-64. The model predictions agree well with experimental observations. Based on the phase field simulation results, fast-acting models are developed for direct industrial applications.

According to experimental observations, texture may play an important role in controlling β grain growth during β-annealing in Ti-64. Texture evolution during grain growth is determined by the interplay among many factors, including the number of texture components, initial fraction, spatial distribution and grain size distribution of each texture component, and the dependences of grain boundary energy and mobility on misorientation. To develop fundamental understanding of the individual and combined effects of these factors on texture evolution and the corresponding effect on grain growth kinetics, we developed a phase field model and carried out a series of simulations with different combination of these factors. The simulation study has suggested that even though all the above mentioned factors affect texture evolution, the key parameter that controls texture evolution is the local grain boundary energy density characterized by γ/D, where γ is grain boundary energy and D is average grain size. This finding simplifies dramatically the process for the development of a fast-acting model for texture-controlled grain growth (Fig. 2.6).
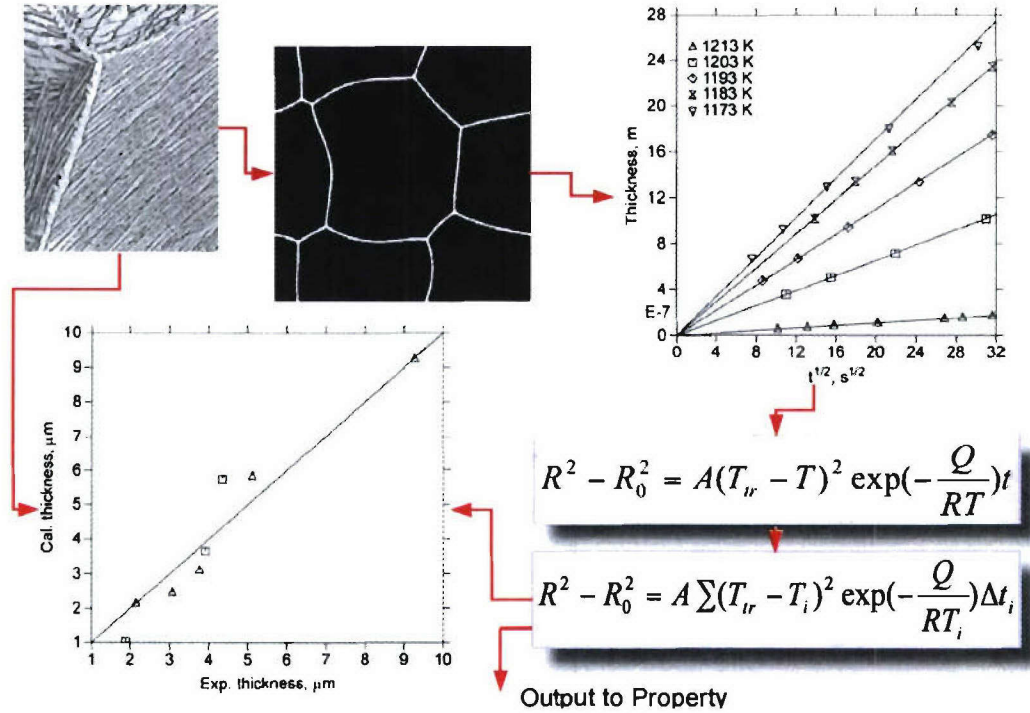
Fig. 2.2. Development of phase field model of grain boundary alpha thickening and formulation of constitutive rate equations based on phase field simulations. Good agreement has been achieved between model predictions and experimental observations.

The equations shown in the figure:

$$R^2 - R_0^2 = A(T_{tr} - T)^2 \exp\left(-\frac{Q}{RT}\right)t$$

$$R^2 - R_0^2 = A \sum (T_{tr} - T_i)^2 \exp\left(-\frac{Q}{RT_i}\right)\Delta t_i$$

Output to Property

Incorporation of effect from spatial distribution

New constitutive equation for globular α

$$f = 1 - \exp\left(-\frac{1}{\xi}\frac{D}{R_f^2}\frac{c_0 - c_\beta}{c_\alpha - c_\beta}t\right)$$
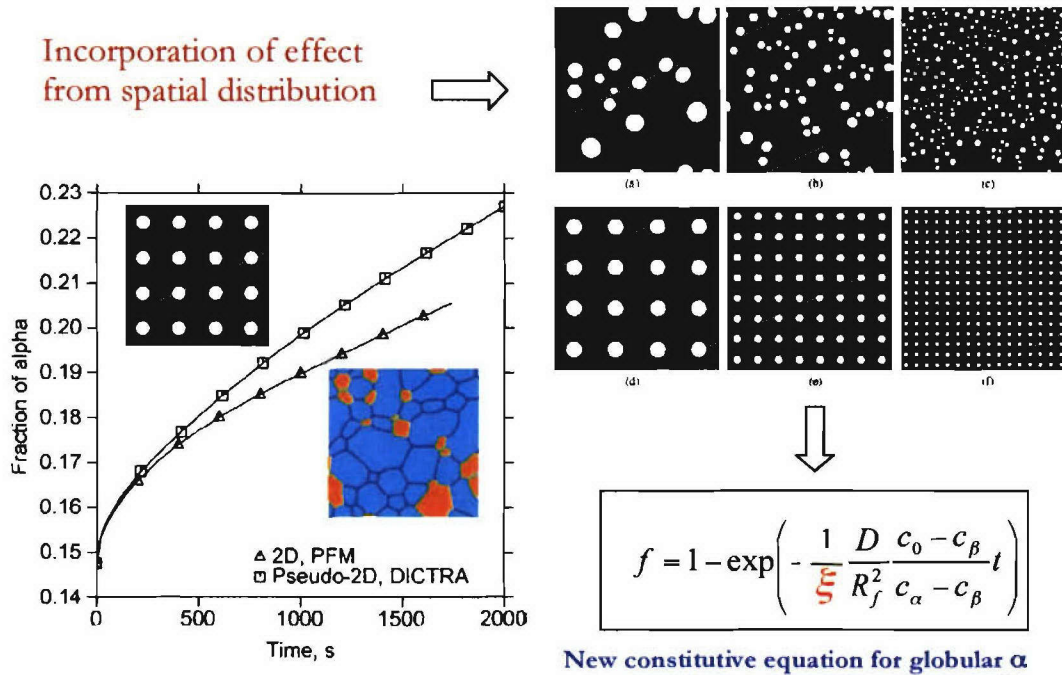
Fig. 2.3. Development of phase field model of growth of globular α and formulation of a constitutive rate equation that incorporates corrections for non-uniform particle size and spatial distribution.
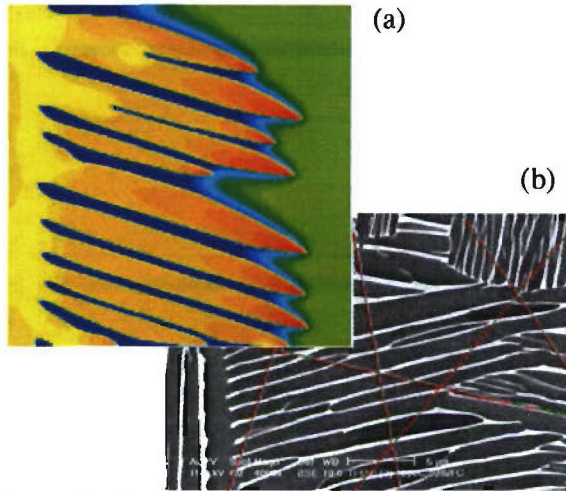
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Fig. 2.4. (a) Formation of sideplates due to interface instability as simulated by the phase field method; (b) experimental observation in Ti-6-4.
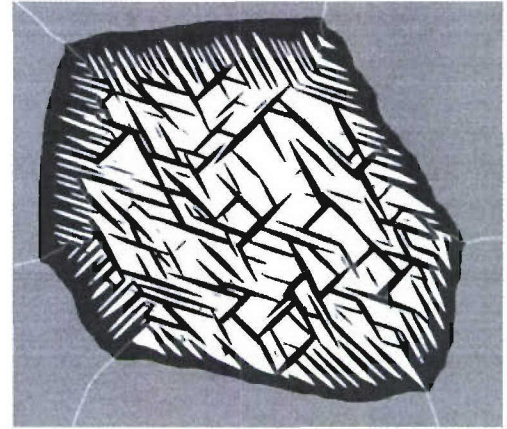

Fig. 2.5. Simulated side plate growth and basketweave structure formation within a six-sided grain by the phase field method.
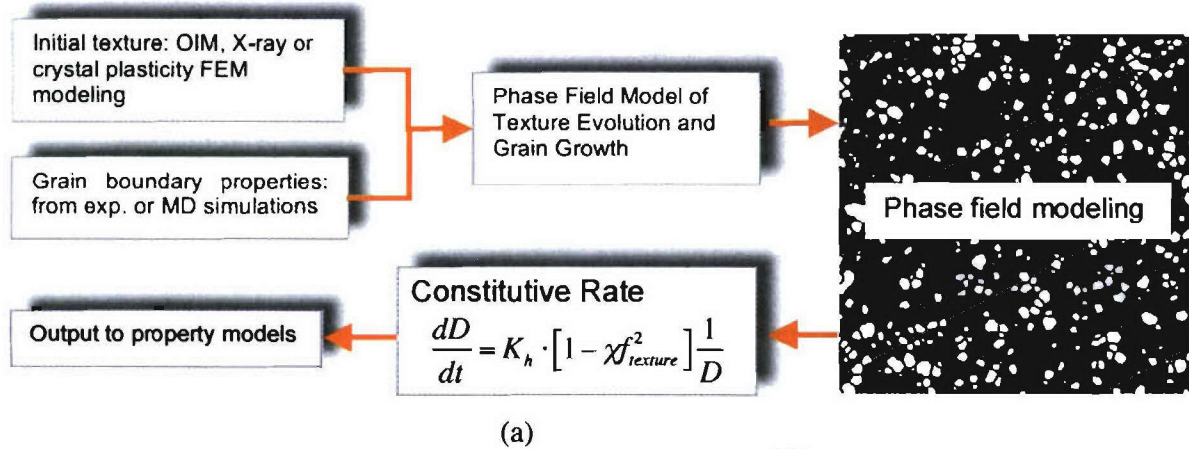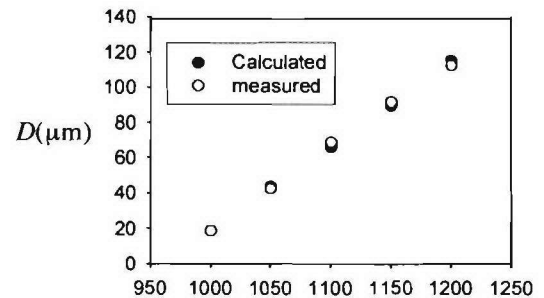

(a)

Fig. 2.6. Development of phase field model of texture evolution during β-annealing and formulation of constitutive rate equation of grain growth, which for the first time incorporates texture effect (a). The constitutive rate equation developed based on the phase field simulations was shown to be successful in predicting β grain growth taking into account texture information in the initial microstructure inherited from previous processing history (b).

In the flow diagram:

- Initial texture: OIM, X-ray or crystal plasticity FEM modeling
- Grain boundary properties: from exp. or MD simulations
- Phase Field Model of Texture Evolution and Grain Growth
- Phase field modeling
- Output to property models

Constitutive Rate

$$\frac{dD}{dt} = K_h \cdot \left[1 - \chi f_{texture}^2 \right] \frac{1}{D}$$

(b)

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Task 3: A Multi-time scale integration method for cyclic deformation in polycrystalline metals

This research project has initiated the development of a accelerated cyclic analysis method, through the introduction of a multi-time scaling time integration in computational models for simulating cyclic deformation. In particular, the model will be used to investigate the effect of material microstructure on deformation behavior and fatigue life of polycrystalline metals and alloys.

Motivation

The mechanical behavior of metals under cyclic loading has great technological importance and significant efforts have been made to predict the fatigue life of these materials. The mechanical behavior of metals under cyclic loading has great technological importance and significant efforts have been made to predict the fatigue life of these materials. The phenomena of high cycle and low cycle fatigue have been traditionally characterized using macroscopic parameters like applied stresses, cyclic frequency, loading waveform, hold time etc., as well as statistical distributions of fatigue life and fatigue strength. Fatigue design by total life approaches includes the stress-life or S-N approach and the strain-life approach e.g. the Coffin-Manson rule. The total life approaches have been adjusted for notch effects using fatigue strength reduction and for variable amplitude fatigue e.g. in the Palmgren-Miner rule of cumulative damage. Alternatively, the defect or damage tolerant approaches determine fatigue life as the number of cycles to propagate a crack from a certain initial size to a critical size. These are determined from threshold stress intensity, fracture toughness, limit load, allowable strain or allowable compliance. Although these models have worked well for alloys under specific test conditions, a lack of underlying physics and microstructure based considerations impede their portability to generic materials and load conditions. The mechanical behavior and fatigue failure response are governed by microstructural features that include morphological and crystallographic characteristics, e.g. crystal orientations and misorientations, grain boundary geometry etc. The recent years have seen significant efforts in modeling cyclic plasticity and fatigue with considerations of microstructural stress-strain evolution. Finite element calculations have shown that depending on the loading conditions, significant gradients of stress can arise within a single grain. Most simulations performed with 3D crystal plasticity are in the range of 100 cycles and the results are subsequently extrapolated for fatigue predictions. In modeling fatigue, it is however desirable to conduct simulations for a significantly high number of cycles to reach local states of damage initiation and growth. Conventional methods of time integration using semi-discretization present numerous challenges due to the variation in time scales ranging from the scale of the entire process to the time resolution required by the damage evolution and crack propagation.

Progress in this Task

In this work, a method of solution of crystal plasticity equations is developed in this paper using multiple time scaling that involves compression and rarefaction of time scales. The method enables large time scale homogenization in relatively benign periods of deformation, to very fine time scale simulations in temporal regions needing high resolution, e.g. with evolving localization. The multi-time scaling is based on

homogenization with the asymptotic expansion method in the time domain for heterogeneous materials including polycrystals. The governing equations are divided into two initial-boundary value problems with two different time scales. One is a slow time scale (t) problem for describing the smooth averaged solution (global problem) and the other is for the remaining oscillatory portion at a fast time scale τ). To solve the constitutive equations, each variable is decomposed into an averaged temporal part and an oscillatory part. The oscillatory variables are expanded.

Solutions are then obtained for each portion and consequently superposed to obtain the full solution. The initial comparisons of single time stepping with multi-time scale methods show a significant promise for this methodology for the class of problems considered. Figure 3.1 shows a comparison of a cyclic deformation problem solved by various methods. Figure 3.1(a) shows the FEM model of a polycrystalline model with the orientation distribution and applied cyclic load. Figure 3.1(b) shows the solution of the problem obtained by a detailed single time scale time integration scheme and a homogenized solution using a compressed slow scale. In figure 3.1(c) a blow up of a region of the plot in 3.1(b) is shown with an additional de-compression effect by adding 0-th order oscillators to the homogenized solution for reverting to the detailed time resolution. The comparison with the reference solution shows excellent accuracy while the efficiency gained through time compression can be enormous (about 50 times the single time scale). The evolution of microscopic variables by the single and multi-time scale methods are shown in figure 3.2. The promise of this technique has been demonstrated in this work.
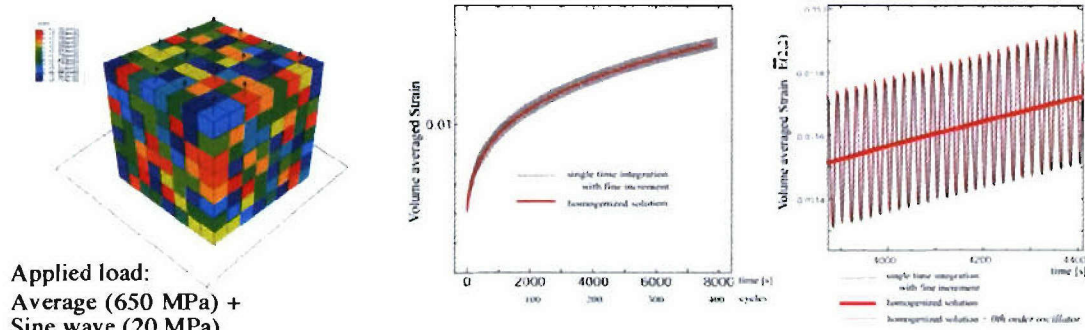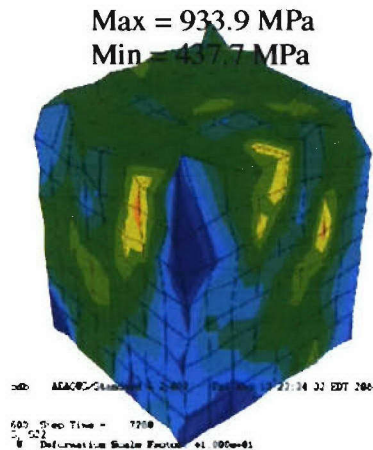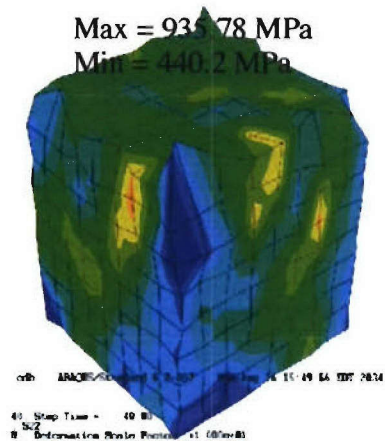

Applied load:
Average (650 MPa) +
Sine wave (20 MPa)

Figure 3.1: Stress-time plots for different time integration methods in cyclic deformation simulation.

Max = 933.9 MPa
Min = 437.7 MPa

σ_{22} distribution in single time integration

Max = 935.78 MPa
Min = 440.2 MPa

σ_{22} distribution in multi-scale time integration

Figure 3.2: Microstructural stress distribution by single and multi-time scale time integration.

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Publications:
1. Y. Wang, N. Ma, Q. Chen, F. Zhang, S.-L. Chen, Y. A. Chang, "Predicting Phase Equilibrium, Phase Transformation, and Microstructure Evolution in Titanium Alloys," JOM, September 2005, pp32-39.

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